Consistent deorbitalization of MVS meta-GGA exchange-correlation functional

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The search for better approximations to the exchange-correlation (XC) energy functional in the Kohn-Sham [1] scheme is still a topic of great interest. Provision of improved approximations would help in achieving more refined descriptions of the chemical and physical properties of important solid systems and their molecular constituents. In 2017 Mejía-Rodríguez and Trickey [2] proposed the deorbitalization of meta-GGA functionals. The basic strategy is to replace the Kohn-Sham kinetic energy density term in such approximations with a term that does not depend upon the KS orbitals but only upon the electron density, its gradient, and its Laplacian. When successful, this procedure makes possible DFT calculations of thermochemical properties with the quality of a meta-GGA functional, but with lower computational cost.

In some cases the deorbitalization strategy does not work. To aid in diagnosis, we studied the deorbitalization of the meta-GGA made very simple (MVS) functional [3]. We tested various reparametrized kinetic energy functionals (deorbitalizers) and reoptimized their parameters using atomic electron densities from the MVS XC functional instead of atomic Hartree-Fock electron densities.

Standard test sets were treated to determine the quality of the various schemes. For molecules those were heats of formation (G3/99X), bond lengths (T96-R), and vibrational frequencies (T82-F). For solids we considered static lattice constants and cohesive energies for 55 systems, bulk moduli for 44, and KS band gaps of 21 insulators and semiconductors. Our results show that the deorbitalized MVS functional (MVS-L) is reasonable for the calculation of these properties while maintaining quality similar to the original functional. Though Ref. DM-SBT found a “best performance” deorbitalizer for MVS when tested against molecular data alone, we do not find that deorbitalization to be equally successful for the solids.

References

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